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AN ACCURATE METHOD FOR EVALUATING THE OVERLAP TERM IN THE UNRESOLVED REGION

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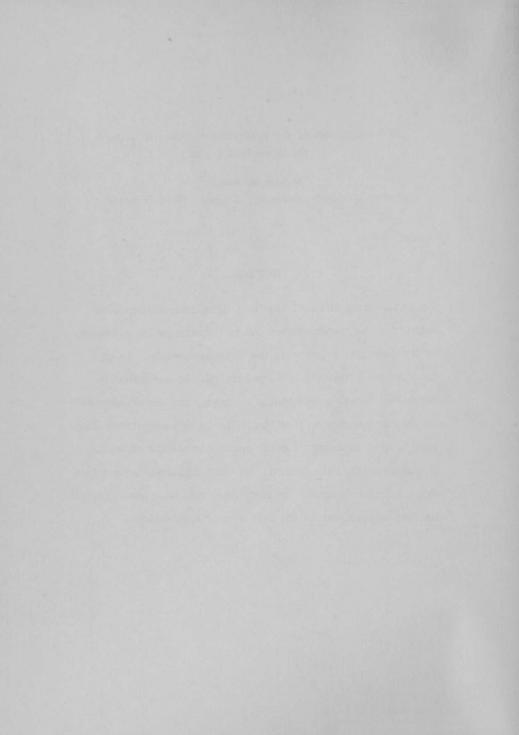
An Accurate Method for Evaluating the Overlap Term in the Unresolved Region

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ABSTRACT

An accurate and efficient method has been developed for estimating the overlap effect due to the neighboring resonances of the same spin sequence in the unresolved region. In contrast to the previously developed method, the new method is capable of treating practically all energy regions of interest in the fast reactor applications. The Dyson's correlation function is used to account for the proper correlation of levels. In the numerical calculations, the exact Doppler-broadened lineshape function is used. The method has been made economical for routine calculations in the fast reactor applications.



I. INTRODUCTION

Extensive studies on the role of the resonance overlap effect in fast reactor calculations have been described in previous work. 1,2 A rather crude method was proposed for estimating the overlap effect of neighboring resonances of the same sequence in the unresolved energy region. This early method is believed to be reasonably accurate in the energy region where resonances are strongly overlapping. However, it becomes questionable in the relatively low-energy region and for the cases where the "equivalent" potential scattering cross section becomes small. These are the situations that one must face in the analysis of Doppler-effect experiments and of heterogeneity studies for critical assemblies. The significance of the overlap effect on the temperature dependence of the Doppler coefficient under meltdown conditions where the extremely high temperature of the fuel pin may be accompanied by spectrum hardening due to the loss of sodium must also be realized. Under this condition, even the well-separated 238U resonances become strongly overlapping. The accurate estimation of the overlap effect is, therefore, important in fast reactor safety studies. Some preliminary results concerning this problem have been given in previous work. Hence, an accurate estimation of the overlap effect is desirable.

The purpose of this report is to describe a newly developed method for estimating the overlap effect due to resonances of the same spin sequence in the unresolved energy region. Improvement on the earlier method 1,2 has been made in three general areas. First of all, the exact Doppler-broadened line-shape function $\psi(\sigma,x)$ is used instead of the approximate Gaussian form used previously. Secondly, the new method is

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made applicable even in the relatively low-energy region and for cases where the equivalent scattering cross sections per absorbing atoms σ_p^{eq} is small. The assumption that $[\psi(\theta,x)/\beta]<<1$ used in the previous method has been avoided. This assumption obviously breaks down whenever $[\psi(\theta,0)/\beta] \leq 0$. Finally, the Dyson's correlation function 4 for levels is used instead of the rather crude approximation used in the previous work. The use of the approximate correlation function described previously was found to underestimate the overlap effect in the high-energy region. 5

The analytical and numerical foundations of the proposed method are described in detail from Section II through Section V. In order to test and evaluate the merits of the proposed method, a code has been developed. Section VI describes the CHOPSUEY code and its computing time required for calculations of practical interest. The listing of relevant subroutines are also given.

II. FORMULATION OF THE OVERLAP TERM

If the NR-approximation and the "nearest neighbor" approximation 1,2 are assumed, the overlap term for a given process x due to the resonances of the same sequence can be written as

$$\tilde{0}_{x} = \frac{1}{\langle D \rangle} \left\langle \frac{\Gamma_{xk}}{2} \int_{-\infty}^{\infty} \Omega(\delta) \frac{d\delta}{\langle D \rangle} \int_{-\infty}^{\infty} \frac{\psi_{k}}{\beta_{k} + \psi_{k}} \frac{A_{k}, \psi_{k}, dx_{k}}{\beta_{k} + \psi_{k} + A_{k}, \psi_{k}} \right\rangle_{k \text{ and } k}, (1)$$

where A_k , is the ratio of the peak cross section of resonance k' with respect to a given resonance k and $\langle D \rangle$ is the average level spacing.

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The brackets $\langle \ \rangle$ indicate the statistical average over the distribution functions of the resonance parameters of both k-th and k'-th resonances. The correlation function $\Omega(\delta)$ is the probability that any k'-th resonance will be found at a distance of δ = E_k - E_k , from a given resonance k. For our purpose, $\Omega(\delta)$ is taken to be Dyson's two-level correlation function. 4,5

$$\Omega(y) = 1 - \{s(y)\}^2 + \frac{\partial s(y)}{\partial y} si(y)$$
, (2)

where

$$y = \frac{\pi |E_k - E_{k'}|}{D}$$
 (3)

$$s(y) = \frac{\sin|y|}{y} \tag{4}$$

and the sine integral si(y) is defined as

$$si(y) = -\int_{y}^{\infty} \frac{\sin t}{t} dt .$$
 (5)

Equation (1) involves multiple integrals. A direct numerical approach is believed to be extremely time-consuming, if at all practical, for routine design calculations. Equation (1) can be simplified considerably by series expansion.

Note that the integral can be expressed as

$$\int_{-\infty}^{\infty} \frac{\psi_{k}}{\beta_{k} + \psi_{k}} \frac{A_{k} \cdot \psi_{k}}{\beta_{k} + \psi_{k} + A_{k} \cdot \psi_{k}} dx_{k} = \int_{-\infty}^{\infty} \frac{\psi_{k}}{\beta_{k} + \psi_{k}} \left\{ \frac{\psi_{k}}{\beta_{k} + \psi_{k}} - \frac{A_{k} \psi_{k} \psi_{k}}{\left(\beta_{k} + \psi_{k}\right)^{2}} + \cdots \right\} dx_{k}$$

provided the resulting integrals are uniformly convergent. The substitution of Eq. (6) into Eq. (1) gives

$$\tilde{0}_{\mathbf{x}} = K_1 - K_2 + \cdots, \tag{7}$$

where

$$K_{1} = \frac{1}{\langle D \rangle^{2}} \langle \Gamma_{xk} J \rangle_{k} \langle \Gamma_{k} J \rangle_{k} - L_{1} , \qquad (8)$$

$$L_{1} = \frac{1}{\langle D \rangle} \int_{-\infty}^{\infty} W \left(\frac{\delta}{\langle D \rangle} \right) \frac{d\delta}{\langle D \rangle} \int_{-\infty}^{\infty} \left\langle \frac{\Gamma_{xk}}{2} \frac{\psi_{k}}{\beta_{k} + \psi_{k}} \right\rangle_{k} \left\langle \frac{\Gamma_{k}}{2} \frac{\psi_{k}}{\beta_{k} + \psi_{k}} \right\rangle_{k} dx_{k} , (9)$$

$$J = \int_0^\infty \frac{\psi_k \, \mathrm{d}x_k}{\beta_{1_k} + \psi_{1_k}} \,, \tag{9a}$$

$$K_{2} = -\frac{1}{\langle D \rangle^{2}} \langle \tau_{xk} \rangle_{k} \frac{\Gamma_{k'}}{2} \sigma_{p}^{eq} \frac{\partial}{\partial \sigma_{p}^{eq}} J_{k'} - L_{2} , \qquad (10)$$

$$\label{eq:L2_loss} L_2 = -\frac{1}{\left\langle D \right\rangle} \int_{-\infty}^{\infty} W \left[\frac{\delta}{\left\langle D \right\rangle} \right] \frac{\mathrm{d}\delta}{\left\langle D \right\rangle} \int_{-\infty}^{\infty} \left\langle \frac{\Gamma_{\mathrm{xk}}}{2} \left[\frac{\psi_{\mathrm{k}}}{\beta_{\mathrm{k}}} - \frac{\psi_{\mathrm{k}}}{\beta_{\mathrm{k}} + \psi_{\mathrm{k}}} \right] \right\rangle_{\mathrm{k}} \left\langle \frac{\Gamma_{\mathrm{k}}}{2} \sigma_{\mathrm{p}}^{\mathrm{eq}} \frac{\partial}{\partial \sigma_{\mathrm{p}}^{\mathrm{eq}}} \frac{\psi_{\mathrm{k}}}{\beta_{\mathrm{k}} + \psi_{\mathrm{k}}} \right\rangle_{\mathrm{k}} \mathrm{d}x_{\mathrm{k}},$$

(11)

$$\tau_{xk} = \frac{\Gamma_{xk}}{2\beta_k} \int_{-\infty}^{\infty} \frac{\psi_k^2}{\beta_k + \psi_k} dx_k = \frac{\pi}{2} \left\langle \frac{\Gamma_{xk}}{\beta_k} \right\rangle - \left\langle \Gamma_{xk} J \right\rangle_k , \qquad (12)$$

$$-\frac{\partial}{\partial \sigma_{p}^{eq}} \left(\frac{\psi_{k}}{\beta_{k} + \psi_{k}} \right) = \left[\frac{\psi_{k}}{\beta_{k} + \psi_{k}} - \frac{\psi_{k}^{2}}{\left(\beta_{k} + \psi_{k}\right)^{2}} \right] \frac{1}{\sigma_{p}^{eq}}, \quad (13)$$

and

$$W\left(\frac{\delta}{\langle D \rangle}\right) = 1 - \Omega\left(\frac{\delta}{\langle D \rangle}\right). \tag{14}$$

For cases of practical interest, the series in Eq. (7) is uniformly convergent on physical grounds. In contrast to the series expansion used in the previous work, it is clear that the terms in Eq. (7) will converge more rapidly even in the relatively low-energy region. In the region where the previous series expansion is valid, Eq. (7) is equivalent to the inclusion of many terms in the previous expression. In the high-energy region, both expressions become identical. The rapidity of convergence of Eq. (7) depends on the degree of the self-shielding effect of the given isotope and the ratio of the average level spacing and the Doppler width in the energy region under consideration. Note that $\langle \tau_{xk} \rangle$ defined in Eq. (12) represents the degree of self-shielding effect and is proportional to $1-\bar{s}$ where \bar{s} is the self-shielding factor

$$\left\langle \Gamma_{\mathbf{x}k}J\right\rangle\!\!\left\langle\!\!\left\langle\frac{\Gamma_{\mathbf{x}k}^{\pi}}{2}\!\right/\!\beta_{k}\right\rangle.$$

In fact, for practically all problems of interest in the unresolved region, the self-shielding effect is relatively small and $\langle \tau_{xk} \rangle$ is generally much smaller than $\langle \Gamma_{xk} J \rangle_k$. From Eqs. (8), (10), and (13), it is obvious that $K_1 >> K_2$ if the self-shielding effect is relatively weak. A similar argument can be made to show that the higher-order terms are also small. It is generally true that the resonance sequence with large average spacing

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will tend to have a stronger self-shielding effect in the low-energy region. It will be shown in a later section that one seldom needs to retain the higher-order terms beyond K_2 and all K_n terms become identically zero when the average spacing $\langle D \rangle$ becomes much larger than the corresponding Doppler width and the average total width.

Since the J-integral and other related integrals can be readily evaluated using the algorithm proposed previously, 6 the main task here is to evaluate the integral L_1 . Once L_1 is known, L_2 can be evaluated quite readily as one will see.

III. EVALUATION OF L1

 L_1 defined in Eq. (9) is still too complicated and a direct numerical approach will undoubtedly require excessive computing time. Furthermore, $W(\delta/\langle D \rangle)$ involves oscillatory functions which are highly undesirable for quadrature formulas. The problem can be resolved by the use of the Fourier transform technique.

A. Technique of Fourier Transform

Define a function $P_k(\xi)$ such that

$$P_{k}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\psi_{k} e^{i\xi x_{k}}}{\beta_{k} + \psi_{k}} dx_{k} = \mathbf{F} \left\{ \frac{\psi_{k}}{\beta_{k} + \psi_{k}} \right\} . \tag{15}$$

The Fourier transform of W($\delta/\langle D \rangle$), say $\omega(\xi)$, is $^{4},^{5}$

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III - EVALUATION OF L.

In defined in Eq. (8) is still too complicated and a direct named—cal approach will undoubtedly require excessive computing than. Furthermore, W(4/(D)) involves oscillatury functions which are highly undosinged by the use of the formular country tomulas. The problem can be resolved by the use of the Fourier country technique.

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From the convolution theorem and the Parseval theorem, 7 it can be shown quite readily that

$$L_{1} = \frac{1}{2\langle D \rangle^{2}} \int_{-\infty}^{\infty} \sqrt{2\pi} \, \omega(\xi) \left\langle \Gamma_{xk} P_{k} \left[\frac{\Gamma_{k}}{2} \, \xi \right] \right\rangle_{k} \left\langle \frac{\Gamma_{k'}}{2} \, P_{k'} \left[\frac{\Gamma_{k'}}{2} \, \xi \right] \right\rangle_{k'} d\xi . \quad (17)$$

Note that the quantities inside the brackets are the statistically averaged values over the appropriate distribution functions of resonance parameters. The same subscript can be used for the two averaged quantities.

It is interesting to note that $\mathbf{F}_k(\xi)$ is the unique solution of the following integral equation

$$\beta_{k} P_{k}(\xi) + \frac{1}{2} \int_{-\infty}^{\infty} e^{-(\xi - t)^{2}/\theta_{k}^{2}} - |\xi - t| P_{k}(t) dt = \sqrt{\pi/2} e^{-\xi^{2}/\theta_{k}^{2}} - |\xi| , (18)$$

where the function on the right-hand side is simply the Fourier transform of the ψ -function as described in Ref. 8.

Before attempting to solve these integral equations, it is important to realize some analytical characteristics of $P_k(\Gamma_k\xi/2)$. First of all,

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from the convolution theorem and the Earsaval theorem, it can be seen quite realily that

$$L_{3} = \frac{1}{2(0)^{6}} \left[\sqrt{2\pi} \, \omega(\epsilon) \left(\epsilon_{10} \rho_{10} \left(\frac{\epsilon_{1}}{2} \, \epsilon \right) \right) \sqrt{\frac{\epsilon_{1}}{2}} \, \epsilon_{10} \cdot \left(\frac{\epsilon_{1}}{2} \, \epsilon_{10} \cdot \left(\frac{\epsilon_{10}}{2} \, \epsilon_{10}$$

Note that the quantities inside the brackets are the statistically averaged values over the appropriate distribution functions of resonance parameters. The same subscript can be used for the two averaged quantities.

In is interesting to note that $F_{\chi}(t)$ is the unique solution of the following interval equation

where the function on the right-hand side is simply the fourier beautions of the 4-function as described in Ref. 8.

Before attempting to solve these integral operions, it is important to realize some analytical characteristics of Px(Fx1/2). First of all,

 $P_k(\Gamma_k\xi/2)$ is an even function so that $P_k(\Gamma_k\xi/2) = P_k(-\Gamma_k\xi/2)$. Secondly, in the limit of large β_k , $P_k(\Gamma_k\xi/2)$ approaches asyptotically to

$$P_{k}\left(\frac{\Gamma_{k}}{2}\,\xi\right) \simeq \sqrt{\pi/2}\,\exp\left(-\frac{\Delta^{2}}{4}\,\xi^{2}\,-\frac{\Gamma_{k}}{2}\,|\xi|\right) / \beta_{k} \quad , \tag{19}$$

where Δ is the Doppler width. Thirdly, in another extreme where Γ_k is large compared to $\Delta,\,\psi$ becomes Lorentzian. As a result, $P_k\Big(\Gamma_k\xi/2\Big)$ approaches

$$P_{k}\left[\frac{\Gamma_{k}}{2} \xi\right] \simeq \frac{\sqrt{\pi/2}}{\sqrt{\beta_{k}(\beta_{k}+1)}} \exp\left[-\frac{\Gamma_{k}}{2} \sqrt{\frac{\beta_{k}+1}{\beta_{k}}} \xi\right], \qquad (20)$$

according to Eq. (15). Of particular academic interest is the fact that Eq. (20) yields

$$L_{1} = \frac{\pi^{2}}{4\langle D \rangle^{2}} \left\langle \Gamma_{xk} \Gamma_{k} \cdot \sqrt{\frac{1}{\beta_{k} \left(\beta_{k} + 1\right)}} \sqrt{\frac{1}{\beta_{k} \cdot \left(\beta_{k} + 1\right)}} \frac{1}{z} \left\{ 1 - \exp(-z) \frac{\sinh z}{z} \right\} \right\rangle_{k \in k}, \tag{20a}$$

where - Ei(-z) is the exponential integral, and

$$z = \frac{\pi}{\langle D \rangle} \left[\Gamma_k \sqrt{\frac{\beta_k + 1}{\beta_k}} + \Gamma_k - \sqrt{\frac{\beta_k + 1}{\beta_k}} \right] / 2.$$
 (20b)

It follows that

Pr(1,672) is an even Amelian to that Pr(1,672) = Pr(-1,672). Secondly, an the light of large I/S Pr(1,672) approaches asymptotically to

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$$K_{1} = \frac{\pi^{2}}{4\langle D \rangle^{2}} \left\langle \Gamma_{xk} \sqrt{\frac{1}{\beta_{k} (\beta_{k} + 1)}} \Gamma_{k} \sqrt{\frac{1}{\beta_{k} (\beta_{k'} + 1)}} \phi_{0}(z) \right\rangle_{k \in k'}, \quad (20c)$$

where $\phi_0(z)$ is identical to that derived by Moldauer 9 for the correction term of the fluctuation in the reaction cross section based on a completely different physical argument. This signifies the strong analogy between these overlap correction terms.

The characteristics defined by Eq. (19) and Eq. (20) provide some clues on how $\left\langle \Gamma_{xk} P_k \left(\Gamma_k \xi/2 \right) \right\rangle$ and $\left\langle \left(\Gamma_k /2 \right) P_k \left(\Gamma_k \xi/2 \right) \right\rangle$ vary as functions of ξ . This information is extremely important in the subsequent construction of quadrature formulas.

With proper normalization, Eqs. (17) and (18) can be evaluated quite readily using Gauss-Hermite quadratures. Define a new variable

$$\eta = \alpha \xi$$
, (21)

where α is set to be

$$\alpha = \sqrt{(\langle D \rangle / \pi)^2 + (\Delta^2 / 2) + \gamma^2}$$

and

$$\gamma = \left\langle \Gamma_k - \sqrt{\frac{\beta_k + 1}{\beta_k}} \right\rangle \tag{22}$$

Equation (17) becomes

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$$L_{1} = \frac{1}{\alpha} \frac{1}{2\langle D \rangle^{2}} \sum_{i=1}^{N} a_{i} \sqrt{2\pi} \omega \left(n_{i} / \alpha \right) \left(\Gamma_{\mathbf{x}k} g_{2} \left(n_{i} \right) P_{k} \left(\frac{\Gamma_{k} n_{i}}{2\alpha} \right) \right)$$

$$\cdot \left\langle \frac{\Gamma_{k}}{2} g_{2} \left(n_{i} \right) P_{k} \left(\frac{\Gamma_{k} n_{i}}{2\alpha} \right) \right\rangle g_{1} \left(n_{i} \right) + R_{N} , \qquad (23)$$

where

$$g_2(n_i) = \exp\left[\frac{\Delta^2 n_i^2}{4\alpha^2}\right]$$
 (24)

$$g_1(\eta_i) = \exp\left[\left(\frac{\langle \underline{D} \rangle^2}{\pi^2 \alpha^2} + \frac{\gamma^2}{\alpha^2}\right) \eta_i^2\right]$$
 (25)

$$a_{n} = \frac{2^{n-1} n! \sqrt{\pi}}{n^{2} \left[H_{n-1} (n_{n}) \right]^{2}}$$
 (25a)

$$R_{N} = \frac{N! \sqrt{\pi}}{2^{N}(2N)!} f^{(2N)}(y) \qquad (-\infty < y < \infty)$$
 (25b)

and n_i is the i-th zero of the Hermite polynomial $H_n(n)$ and $f^{(2n)}(y)$ is the 2n-th derivatives of the integrand. Here, the purpose of changing the variable is to ensure that the integrand varies slowly as a function of n in order to make the Gauss-Hermite quadrature highly efficient regardless what values of $\langle D \rangle$, Δ , Γ_k , or β_k are. Similarly, the integral in Eq. (18) can be replaced by the Gauss-Hermite quadrature so that the resulting equation assumes a matrix equation of the form

$$AP = B . (26)$$

and a, for the 1-th sero of the Henrich polynomial H₁(n) and f⁽²ⁿ⁾(y) is the he-th description of the integrand varies slowly as a function of a in order to make the Sausa-demilts quadrature identy efficient requirement values of (D), A, C, or S, are: Similarly, the intemal in Eq. (18) can be replaced by the Gausa-Hamilte quadrature to that the resulting equation essues a actrix equation of the form

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By normalizing each row of the matrix element of A to its diagonal element, one has

$$A_{ij} = \frac{a_{j}}{\mu_{\alpha}} g_{1}(n_{j})g_{2}(n_{j})\Gamma_{k} \exp \left[\frac{\Delta^{2}}{2\alpha^{2}} n_{i}n_{j} - \frac{\Gamma_{k}}{2\alpha} |n_{i} - n_{j}|\right] / N_{0}$$
for $i \neq j$ (27)

and

$$A_{ij} = 1$$
; for $i = j$, (27a)

where

$$N_0 = g_2(n_i) \cdot \left[\beta_k + \frac{a_i r_k}{4\alpha} \cdot g_3(n_i) \right]$$
 (28)

$$g_3(\eta_i) = \left[g_2(\eta_i)\right]^2 \cdot g_1(\eta_i) \tag{29}$$

$$B_{i} = \sqrt{\pi/2} \exp \left(-\frac{\Gamma_{k}}{2} \left| \frac{\eta_{i}}{\alpha} \right| \right) / N_{0} . \tag{30}$$

Hence, the quantities $P_k(\Gamma_k n_i/2\alpha)$ needed for Eq. (23) are just the solution of a system of N equations. An efficient matrix inversion routine is needed for this purpose. The matrix $\bf A$ can be further simplified by partition utilizing the symmetric properties of P_k . The detailed discussion will be given in the next section. It should be noted that the normalization of the matrix proposed here is extremely important from a

By normalizing sees was of the metrols element of A to its diagonal elements one has

$$\sum_{n=1}^{\infty} \frac{1}{n!} \left[(n_1)^n e_1(n_2)^n e_2(n_2)^n e_2(n_2) - \frac{n_2}{2n} (n_2 - n_2) \right] = 0$$

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Herrs, the quantities P₁(P₁n₁/2n) needed for Dq. (D3) are just the solution of a system of a system. As equations. An efficient mixed lawer on hourse of heather simplified By partition stillising the symmetric properties of P₁. The detailed discussion will be given in the next section. It should be noted that the correlated on the months proposed here is extremely incorrect from a

numerical point of view. This ensures that the coefficients of each linear equation will not have vanishingly small magnitudes simultaneously.

From Eq. (23) and Eq. (18), it is clear that the Gauss-Hermite quadrature is most efficient and accurate when the Doppler width is larger than or comparable to the average spacing and the average total width. On the other hand, the Gauss-Hermite quadrature is less efficient when Δ becomes small. Under the latter condition, $P_k \left(\Gamma_k \xi/2 \right)$ approaches the exponential form defined by Eq. (20). From a practical point of view, the proposed quadrature is highly desirable because it yields accurate values for cases with large Doppler width where the relative importance of the overlap effect is high. For the cases with small Doppler width where the overlap effect is less important, the accuracy of the results is less critical. It was found that a 10-point Gauss-Hermite quadrature is sufficient to give accurate results.

Since the matrix inversion of a relatively large matrix is generally time consuming, it is, therefore, desirable to optimize the proposed method to suit the routine application.

IV. ECONOMIZATION

The proposed method can be made more economical in two general areas: (1) in the region where β_k is much larger than $\psi \left(\theta_k, 0\right)$, the matrix inversion can be avoided completely; and (2) in the region where the matrix inversion is necessary the matrix \boldsymbol{A} can be partitioned into four submatrices of the size N/2 × N/2 where N is chosen to be 10 or any even number. The symmetry properties of $P_k \left(\Gamma_k ^n {}_i / 2\alpha\right)$ can be utilized.

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quidrature to most efficient and accommon steen the coppler which is settled. On the comparable to the average specing and the desired cotal. And the other hand, the Gauss-Harmita quadrature is less efficient when a become small. Under the latter condition, P. [1,7/2] approunted the experiential furn defined by Eq. (20). Into a practical rate of the experient of the proposed quadrature is highly desirable because it yields about our time walls about a relative input turns of the eventual office is high. For the coses with small begins and the same the eventual of the coses with a latter than the eventual of the eventual that is not inscribed in a latter than the same of the eventual of the results.

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1. Asymptotic Region
$$\frac{\beta_k + \psi(\theta_k, 0)}{\psi(\theta_k, 0)} \ge 2.5$$

As discussed previously, 6 the quantity $\psi_k/\left(\beta_k+\psi_k\right)$ can be represented by a uniformly convergent series

$$\frac{\psi_{k}}{\beta_{k} + \psi_{k}} = \frac{\psi_{k}}{\beta_{k} + \rho} + \frac{\psi_{k} \left(\rho - \psi_{k}\right)}{\left(\beta_{k} + \rho\right)^{2}} + \cdots, \tag{31}$$

where the parameter ρ can be chosen so that the resulting integrals converge rapidly. One way of choosing ρ is to set

$$\rho = \frac{\int_0^\infty \psi_k^2 dx}{\int_0^\infty \psi_k dx} = \frac{1}{2} \psi \left(\sqrt{2} \theta_k, 0 \right). \tag{31a}$$

By substituting Eq. (31a) into Eq. (15), it can be shown quite readily 5,8 that

$$P_{k}\left(\frac{\Gamma_{k}}{2} \xi\right) \simeq \sqrt{\pi/2} \exp \left[-\frac{\Delta^{2}}{4} \xi^{2} - \frac{\Gamma_{k}}{2} |\xi|\right] \cdot Q(\xi) / \left(\beta_{k} + \rho\right) + \cdots, (32)$$

where

$$Q_{k}(\xi) = 1 + \{\rho - U\}/\{\beta_{k} + \rho\}$$
(33)

$$U = \frac{\theta\sqrt{\pi}}{2\sqrt{2}} \left[\exp\left(\frac{\Delta|\xi|}{2\sqrt{2}} + \frac{\theta}{\sqrt{2}}\right)^2 \operatorname{Erfc}\left(\frac{\Delta|\xi|}{2\sqrt{2}} + \frac{\theta}{\sqrt{2}}\right) + \exp\left(\frac{\Delta^2\xi^2}{8}\right) \operatorname{Erf}\left(\frac{\Delta|\xi|}{2\sqrt{2}}\right) \right], (33a)$$

and Erfc(x) and Erf(x) are the complementary error function and error function, respectively. These functions along with $\psi(y,0)$ can be evaluated by using the exceedingly efficient rational approximation as suggested by Hastings. 10

It is interesting to note that Eq. (31a) serves dual purposes. First of all, it implies

$$Q_{\nu}(0) = 1 \tag{33b}$$

according to Eq. (33). Secondly, the magnitude of the next higher-order term at ξ = 0 assumes a minimum value as readily seen by differentiating with respect to ρ . Since $\omega(\xi)$ defined in Eq. (16) is a rapidly decreasing function of ξ and varies approximately exponentially

$$\omega(\xi) \sim \frac{\langle D \rangle}{\sqrt{2\pi}} \exp \left[-\frac{\langle D \rangle}{\pi} |\xi| \right],$$
 (33c)

the choice of ρ in Eq. (31a) amounts to minimizing the error involved by ignoring the next higher-order term and maximizing the range of validity of Eq. (32) in evaluating L_1 . It was found by numerical experimentation that the validity of Eq. (32) when used in evaluating L_1 can be extended down to

$$\frac{\beta_{k} + \psi(\theta_{k}, 0)}{\psi(\theta_{k}, 0)} \geq 2.5.$$

Approximately 75% of the s-wave and practically all of the p-wave unresolved resonances of the fissile isotopes belong to the asymptotic region. Since Eq. (32) avoids the use of the matrix inversion routine, it represents a significant saving in computing time especially when the fissile isotopes are considered. For fertile isotopes, the asymptotic region for s-wave resonances is much smaller than that for fissile isotopes even though practically all p-wave resonances still belong to this region. It should be noted that, in the absence of the fission-width distribution, the computing time is generally negligible even if the matrix inversion method is used for all mesh points.

2. Non-asymptotic Region

Outside the asymptotic region, accurate calculations can be made by using the matrix inversion technique. Since all quantities inside the summation sign of Eq. (23) are symmetric with respect to η_i = 0, only N/2 terms are needed. However, the kernel that appears in Eq. (18) is not symmetric with respect to the variable of integration. Hence, it is still necessary to invert a N × N matrix even though only half of the vectors $P_k(\eta_i)$ are needed in Eq. (23). The inversion of a matrix with relatively large dimension generally requires an excessive amount of computing time. One way of minimizing the computing time required is to reduce the size of the matrix analytically beforehand. This can be done quite readily by partitioning the matrix $\bf A$ into four submatrices.

Assume the inverse $A^{-1} = E$. It is clear that

$$\mathbf{A}\mathbf{A}^{-1} = \begin{pmatrix} A_{11}A_{12} \\ A_{21}A_{22} \end{pmatrix} \begin{pmatrix} E_{11}E_{12} \\ E_{21}E_{22} \end{pmatrix} = \mathbf{I} , \qquad (34)$$

where I is the identity matrix. Since the Gauss-Hermite weights and mesh points can be arranged in such a way that

$$A_{11} = A_{22} (35)$$

$$A_{21} = A_{12}$$
 (36)

it follows from Eq. (34) that

$$E_{11} = \left(A_{11} - A_{12}A_{11}^{-1}A_{12}\right)^{-1} \tag{37}$$

$$E_{12} = -A_{11}^{-1}A_{12}E_{22} (38)$$

$$E_{22} = E_{11}$$
 (39)

$$E_{21} = E_{12}$$
 (40)

Hence, in the actual numerical calculation, only two N/2 \times N/2 matrix inversions are necessary instead of a N \times N matrix. Since the computing time required for the matrix inversion approximately varies as the cube of the dimension N, a considerable saving in computing time may be achieved if the computing time for the additional matrix algebra in Eqs. (37) and (38) can be minimized. Once E_{11} and E_{12} are known, the vector \boldsymbol{P} is simply

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$$\mathbf{P} = \begin{pmatrix} \mathbf{E}_{11}\mathbf{E}_{12} \end{pmatrix} \begin{pmatrix} \mathbf{B}_{1} \\ \mathbf{B}_{2} \\ \vdots \\ \mathbf{B}_{N} \end{pmatrix} . \tag{41}$$

Further economization may be made on physical grounds. In the low-energy region where the average spacing becomes much larger than the Doppler width and the average natural width, $\omega(\xi)$ in Eq. (17) approaches a Dirac delta function and L_1 becomes

$$L_1 \sim \frac{1}{\langle D \rangle^2} \langle \Gamma_{xk} J \rangle_k \langle \frac{\Gamma_k}{2} J \rangle_k$$
 (41a)

The quantity K_1 vanishes. Similarly, the higher-order terms will also vanish. Hence, it is possible to set K_n = 0 whenever $\langle D \rangle / \Delta$ and $\langle D \rangle / \langle \Gamma \rangle$ become larger than certain values. The proposed method was found to be sufficiently fast that the latter condition for the limiting case is not needed.

V. ESTIMATION OF L2

The second-order term L_2 can be estimated using the same technique discussed previously. Equation (11) can be written as

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The quantity My vanishes. Similarly, the higher-order terms will slad yanish. Hence, it is possible to set My = N sheaver (D)AN entitle Manner larger than certain values. The proposed method whe Diand to De saidlifetently fast that the latter condition for the lamiting year is not needed.

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The second-order term to can be exclusive using the edit technique incommend providencies. Equation (11) can be written as

$$L_{2} = -\frac{1}{2\langle D \rangle^{2}} \int_{-\infty}^{\infty} \sqrt{2\pi} \, \omega(\xi) \left\langle \Gamma_{xk} \left\{ \sqrt{\pi/2} \frac{\exp\left[-(\Delta^{2}\xi^{2}/4) - \left(\Gamma_{k}|\xi|/2\right)\right]}{\beta_{k}} - P_{k} \left(\frac{\Gamma_{k}}{2} \xi\right) \right\} \right\rangle_{k}$$

$$\cdot \left\langle \frac{\Gamma_{k}}{2} \, \sigma_{p}^{(eq)} \, \frac{d}{d\sigma_{p}^{(eq)}} P_{k} \left(\frac{\Gamma_{k}}{2} \xi\right) \right\rangle_{k} d\xi . \tag{42}$$

It is interesting to note that the only unknown in Eq. (42) is the quantity

$$\frac{\mathrm{d}}{\mathrm{d}\sigma_{\mathrm{p}}^{(\mathrm{eq})}} \, P_{\mathrm{k}} \left(\frac{\Gamma_{\mathrm{k}}}{2} \, \xi \right) \, .$$

The latter quantity can be related to $\mathsf{P}_k \Big(\mathsf{\Gamma}_k \xi/2 \Big)$. Let

$$R = -\sigma_{p}^{(eq)} \frac{\partial}{\partial \sigma_{p}^{(eq)}} P\left(\frac{\Gamma_{k}}{2} \xi\right). \tag{43}$$

Differentiating Eq. (18) with respect to $\sigma_p^{(eq)}$ and replacing the integral by the Gauss-Hermite quadrature, one obtains a matrix equation of the form

$$AR = V/N_0 , \qquad (44)$$

and

$$V_{i} = P_{i} \cdot \exp \left[\frac{\Delta^{2} n_{i}}{4\alpha^{2}} \right] \cdot \beta_{k} , \qquad (44a)$$

where P_i is simply the solution of Eq. (26), and N_0 is the normalization factor defined by Eq. (28). Hence,

it is interesting to note that the only unknown in Eq. (42) is the quantity

is larger quantity can be related to Profit [17]. Let

$$-\left[3\frac{1}{3^{2}}\right]q\frac{\left(99\right)_{05}}{6}\left(99\right)_{0}=-32$$

Differentiating Eq. (18) with respect to open and regionize the inve-

where Pr is risply the counties of Eq. (26), and No is its straightfulland in the straightfulland as the straightf

$$R = A^{-1}V/N_0, \qquad (45)$$

where A^{-1} has already been obtained in evaluating L_1 . Thus, the second-order term can be obtained readily once the first-order term is known.

For the cases where the asymptotic formula is applicable, R is simply

$$R_{k}\left[\frac{\Gamma_{k}}{2} \xi\right] = \sqrt{\pi/2} \exp\left[-\frac{\Delta^{2}}{4} \xi^{2} - \frac{\Gamma_{k}}{2} |\xi|\right] \left\{\frac{1 + 2\left[\rho - U_{k}(\xi)\right] / \left(\beta_{k} + \rho\right)}{\left(\beta_{k} + \rho\right)^{2}}\right\} \cdot \beta_{k},$$
(46)

where $\mathbf{P}_{\mathbf{k}}$ and U are defined in Eq. (32) and Eq. (33a).

The same technique, in principle, can be extended to even higher-order terms. However, the evaluation of higher-order terms beyond the second order is believed to be unnecessary on physical grounds. For cases in the low-energy region where the self-shielding effect is large, the average spacing is generally much larger than the corresponding Doppler width and the natural width for all problems of practical interest. Under such conditions, all K_n terms vanish as $\omega(\xi)$ approaches the Dirac δ -function.

VI. CHOPSUEY CODE

In order to test and evaluate the merits of the proposed method, the CHOPSUEY code has been developed. The code uses the input and output routines of the RP-270 code written by Rago¹¹ with modifications to allow for both s- and p-wave resonances. Ten quadrature points were used for

both the neutron width and the fission width distributions. The fast J-integral routine developed recently was incorporated. The statistical averaging and the calculation of the overlap terms are performed in the subroutine UNGRES and UNRES for the fissile and fertile isotopes, respectively. The effective cross sections for both s- and p-wave contributions are given separately in the output. In these subroutines, the average quantities $\langle \Gamma_X J \rangle$, $\langle \Gamma J \rangle$, $\langle \Gamma_X \int_0^\infty \left[\psi/(\beta + \psi) \right]^2 dx \rangle$ and $\langle \Gamma \int_0^\infty \left[\psi/(\beta + \psi) \right]^2 dx \rangle$ are calculated first. In the calculation of $P_k \left(\Gamma_k \xi_1/2 \right)$, the code examines whether the k-th mesh point belongs to the asymptotic region or not. For the points that do not belong to the asymptotic region, a matrix inversion routine is called. The matrix inversion routine was written by Garbow using the Jordan method. A FORTRAN listing of the relevant subroutines are listed in the Appendix.

One of the great concerns is whether the proposed method is efficient enough to be economical in routine applications. Test calculations have been made for problems with ²³⁹Pu and ²³⁸U using ENDF/B parameters. For fertile isotopes, computing time is generally negligible. The most severe test is believed to be the case when ²³⁹Pu is in high concentration. In the calculation of ²³⁹Pu cross sections, not only the averaging over the fission width distribution function is required, but also there are as many as 30 energy points for all five spin sequences. Two cases at room temperature were considered in the test calculations.

Case 1

239Pu:
$$\sigma_{p}^{(eq)} = 71.6/atm$$

238U: $\sigma_{p}^{(eq)} = 40 b/atm$

both the mentron width and the fluctor width distributions. The face J-integral routing developed recently was incorporated. The statistical and averaging and the calculation of the coeffic terms are perfected in the submattine UNIXES and UNIXES for the flexible and fartile isotopes, we expectively. The effective gross sections for both s- and p-sourcement reliabilities or given separately in the output. In these submattine, the average quantities (T.J., (W), (T.J.) is/is : a)) and and

(* [, [w/(8 + x)]² dx) are calculated (i.e., in the calculation of), [, [, [, [, 2]], the code exempts to the early points that do not belong to the separatoric region, a satural inversion couldness in called. The matrix inversion routine is called. The matrix inversion routine was written by Carbon wing the idudes method. A TURTIME Lieux interesting the idudes method. A TURTIME Lieux in the specialist.

One of the great concerns in whether the proposed method is estimient and anough to be economical in routine applications. Next calculations have been made for problem with ""Fu and """ using Sigh's parameter. For invite lactopes, computing time is generally negligible. The mean severe test is believed to be the case when "" In its in high concenture tion. In the calculation of "" " usual series, not only the exercising over the first on what function is required, but also there are not the many as 30 energy points for bit five epin sequences. Not case at now temperature were considered in the turn calculations.

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$$\frac{239 \text{Pu}}{\text{p}}$$
: $\sigma_{\text{p}}^{(\text{eq})} = 300 \text{ b/atm}$

$$\frac{238\text{U}}{\text{p}}$$
: $\sigma_{\text{p}}^{\text{(eq)}} = 30 \text{ b/atm}$

It should be noted that the calculations require much less time at higher temperatures as more entries to the asymptotic region become evident. Table I summarizes the results of the computer time required for the proposed method as compared to the time required for the old MC² routine ¹³ (Subroutine QFJ) without the overlap effect. The time estimates given in Table I include the input-output time as required by the CHOPSUEY code but exclude the compilation time and wait time.

From Table I, it is clear that the proposed method is much superior to the old subroutine not only on the theoretical ground but also in terms of the computing time. The significant improvement in the algorithm for evaluating the generalized J-integral discussed previously is more than enough to compensate for the computing time required for the more rigorous treatment of the overlap effect.

TABLE I
Timing of CHOPSUEY

	sec
MC ² (QFJ) (no overlap)	120
Proposed algorithms (overlap included)	
Case I	47
Case II	28

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   IMPLICIT REAL*8 (A-H, U-Z)
                                                                           A-1
   REAL*4 11, T2, T3, T4, TT0, ITJ, DD
   CUMMON / UFJ1/ZETA, TOT2, BETA, PS1Z, PS1Z2, PS3
   CJMMON/TRTI/TR(62,62), TI(62,62), AIMW, AX, REW, WHY, KI
   CUMMUN/H/TEST1, TEST2, HH
   CUMMUN/SEC/TUT3, THT4
   CUMMON/F/AKI, DEN, RAT, C, AAA
   CUMMON/R/ EERFC, AKG
   CHMMUN/PP/ LL, LP, MU, NCS, IGEDM, NU, NOVLP
   COMMON/DP/ X,
                      E, GMNZ, G, T, UNR, AZFRO, D, C4, ABAR, SIGPO, DZERO,
  ITITLE, C3,CC,Y,UMRGM,UNRG,C1,C2,RAD,FLUXCT,CAP,FISS,SIGP
   DIMENSION X(10), E(100), UNR(100), TITLE(12), Y(10), UNRGM(100)
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  1UNR.G (100)
                                                                                    8
   DIMENSION XXX(10), GN(10), GF(10)
   DIMENSION A(10,10), B(10,100), E1(20), E2(20), AVGGMT(20), AVGFMT(20),
  XA/GTMT(20), DUMMY(10,100), SI(20), E3(20), E4(20)
   DIMENSION FLUXCI(100), CAP(100), FISS(100)
                                                                                    9
                                                                            DOP
                                                                                   11
   DIMENSION YY(10), NW(10)
                                                                            DOP
   DIMENSION GGF(100), GGM(100), TZETA(100), PPSIZ(100), H(100), GGFF(100)
  x, GGMM(100), 88(100), 388(100)
   DIMENSION DUM1(0,10), DUM2(5,5), DUM3(5,5), DUM4(5,5), DUM6(5,5),
  XBP(10,1), VECT(10,1), DUM5(5,5), S(5,5)
   DIMENSION VECT2(10), DUMMY2(10,100), ANDRM(10), BING(10), BINF(10),
  XBINT(10), AVT1(10)
   DIMENSION TIZETA(100)
   DATA YY/3.436159118,2.532731674,1.756683649,1.036610829,
  x,3429013272,-3.435159118,-2.532731674,-1.756683649,-1.036610829,
  x-.3429013272/
   DATA WW/.7640432855D-5,.1343645746D-2,.3387439445D-1,.2401386110,
  x.6108626337,.7640432855D-5,.1343645746D-2,.3387439445D-1,.24013861
  X1,.6108626337/
   DATA E3/.134213820106,.610775665303,.218879759502,.292870987601,
   X.1124773U9201/
                                                                                   32
                                                                            DOP
   DU 2 1=1,NCS
                    100, SIGHI, SIGM2, GMGM, GMF
   READ
                                                                            DOP
                                                                                   34
100 FURMAT (5E12.5)
                                                                            DOP
                                                                                   35
   51GP=C4+51GM1+51GM2
                                                                            DOP
                                                                                   36
   GFRARJ=0.
                                                                                   37
                                                                            DOP
   BARJ=0.
                                                                            DOP
                                                                                   38
   TBARJ=0.0
   THARJZ=0.
   SEG=U.
   SEF=O.
   SET=0.
   FG=0.
                                                                            DOP
                                                                                   76
   FF=0.
                                                                                   77
                                                                            DOP
   F1=0.
   FU2=0.
   F1-2=0.
   F12=U.
   SKE=DSQKT(E(I))
                                                                            DOP
                                                                                   40
   DELTIN=C3/SRE/2.
   I I = 0
   11=0
   AVIND=0.
   AVINDF=0.
   AVINDT=0.
   AVO=O.
   TI=TLEFT(DD)
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GD TU 911 999 XXX(19=1.630645:-1 XXX(2)=1.630645:-1 DDP 51 XXX(2)=2.6842211-1 DDP 52 XXX(4)=4.317/435-1 DDP 53 XXX(4)=4.317/435-1 DDP 54 XXX(5)=5.992173:-1 DDP 55 XXX(7)=1.053244 DDP 56 XXX(7)=1.053244 DDP 57 XXX(8)=1.993041 XXX(9)=1.916293 XXX(10)=3.302585 CR(J)=6,402 **SRE*XXX(J)*V P1 DN 1 K=1,10 CF(K)=6,44*X(K) DDP 63 ZETA=GAM*VELTIN SIGZ=2.656*G*GN(J)/ E(1)/GAM BETA=SIGP/SIGZ AVIND=AVIND+G(K)/EETA AVIND=AVIND+AVIND+G(K)/EETA AVIND=AVIND+ART(6;TA+1.)/BETA) APA=GAM*VERTOF(8;TA+1.)/BETA) APA=GAM*VERTOF(8;TA+1.)/BETA) APA=GAM*SORT(8;TA+1.)/BETA) APA=GAM*SORT(8;TA+1.)/BETA GGF(1)=GF(K) GGMM(1)=GAM* TIZETA(11)=ZETA GUT 11 BUS 11=EETA GGF(1)=GAM* TIZETA(11)=ZETA GUT 12 GGF(1)=GAM* TIZETA(11)=ZETA GUT 13 GUT 14 BUS 13=BTA GGF(1)=GAM* TIZETA(11)=ZETA GUT 14 BUS 13=BTA GGF(1)=GAM* TIZETA(11)=ZETA GUT 15 GUT 16 GGF(1)=GAM* TIZETA(11)=ZETA GUT 16 GGF(1)=GAM* TIZETA(11)=ZETA GUT 17 GUT 18 BUS 13=BTA GGF(1)=GAM* TIZETA(11)=ZETA GUT 18 GUT 19-BTA GUT 19-				
999 xxx(1)=5,175533i=2				
XXX(2)=1.630645:-1 XXX(4)=2.81421t-1 DDP 53 XXX(4)=2.81743t-1 DDP 53 XXX(4)=4.31743t-1 DDP 53 XXX(5)=5.99217dt-1 DDP 56 XXX(7)=1.053244 DDP 57 XX(8)=1.393041 DDP 57 XX(8)=1.393041 DDP 58 XXX(9)=1.916293 DXX(10)=3.302585 DDP 60 GN(J)=GANZ **SRE*XXX(J)*V 91 DN 1 K=1.10 GAM=DON(J)+GF(K)+GAGM ZETA=GAM*VELTIN SIGZ=2.666*GF(N)J/ E(1)/GAM BETA=SIGP/SIG2 AVIND=AVIND+GF(K)+GETA AVINDF=AVIND+GF(K)-GETA AVINDF=AVIND+GF(K)-GETA AVINDF=AVIND+GF(K)-GETA AVINDF=AVIND+GF(K)-GETA AVINDF=AVIND+GF(K)-GETA AVINDF=AVINDF+GF(K)-GETA AVINDE=AVINDF+GF(K)-GETA AVINDE-AVINDF+GF(K)-GETA AVINDE-AVINDF-GF(K)-GETA AVINDE-AVINDF+GF(K)-GETA AVINDE-AVINDF+GF(K)-GETA AVI	000			
XXX(3)=2.884221+-1 XXX(5)=5.992178(-1 XXX(5)=5.992178(-1 XXX(5)=5.992178(-1 XXX(6)=8.00573E-1 XXX(8)=1.930041 DP 56 XXX(8)=1.930041 DP 57 XXX(8)=1.930041 DP 58 XXX(10)=3.302585 DR (J)=6M12-5NE*XXX(J)*V 91 DU 1 K=1.10 GF(K)=GM**Y(K) GF(K)=GM**Y(K) GF(K)=GM**Y(K) GF(K)=GM**Y(K) GF(K)=GM**Y(K) GF(K)=GM**Y(K) GF(K)=GM**Y(K) GF(K)=GM**X(G)=FM**X(G	777			100
XXX(4)==,317/43E=1 XXX(6)==,902/78E=1 XXX(6)==,902/78E=1 XXX(6)==,005/3E=1 XXX(7)=1,0532x4 XXX(9)=1,3930x4 XXX(9)=1,3930x4 XXX(9)=1,3930x4 XXX(9)=3,302585 XXX(1)=3,302585 XXX				
XXX(0)=8.005/3E-1 XXX(7)=1.053244 XXX(8)=1.393041 XXX(9)=1.916293 XXX(10)=3.302585 ROP 59 XXX(10)=3.302585 ROP 59 XXX(10)=6N0Z *SRE*XXX(J)*V 91 DU 1 K=1>10 66 (K)=6M**Y(K) ROP 63 GAM=RON(J)+6F(K)+6-GM ZETA=GAM*DELTIN SIGZ=2.0c6*G*GRI(J)/ E(1)/GAM BETA=SIGP/SIGZ AVIND=AVIND+1-/BETA AVIND=AVIND+6F(K)+6F(B) AVIND=AVIND+FG(K)/EETA AVIND=AVIND+FG(K)/EETA AVIND=AVIND+FG(K)/EETA AVIND=AVIND+FG(K)/EETA AVIND=AVIND+SIGZ AVIND=AVIND+FG(K)/EETA AVIND=AVIND+SIGZ AVIND=AVIND+FG(K)/EETA AVIND=AVIND+FG(K)/EETA AVIND=AVIND+FG(K)/EETA AVIND=AVIND+GG(B,TA+1.)/BETA) AVQ=AVQ+AAAQ CALL FH FFFEIDZ FFFEI		XXX(4)=4.317/43E-1		
XXX(7)=1.353244 XXX(8)=1.393041 XXX(9)=1.916293 XXX(10)=3.302585 GN(J)=GMNZ #SRE*XXX(J)*V 91 DU 1 K=1:D G+(K)=GM+*Y(K) GAM=GN(J)+GF(K)+GMGM ZETA=GAM*DELTIN SIGZ=2.6-6*G*GN(J)/ E(1)/GAM BETA=SIGP/SIGZ AMINDF=AVIND+1./GETA AMINDF=AVIND+1./GETA AMINDF=AVIND+1./GMNBETA AMINDF=AVIND+1./GMNBETA AMAQ=GAM*DSQRT((BETA+1.)/BETA) AMAQ=GAM*DSQRT((BETA+1.)/BETA) AMAQ=GAM*DSQRT((BETA+1.)/BETA) AMAQ=GAM*DSQRT((BETA+1.)/BETA) IF (NUWLP.NE.O.)GO TO 6 THAR JZ=TBAR JZ=FJP-Z*GAM TEST1=(BETA+SIZ)/PSIZ II (IEST1-GE.2.5)GO TO 5 II=II+1 BBG(I)=BETA GGF(I)=GF(K) GGMM(I)=GAM TYETA(I)=ZETA GU TU 6 JUBJJ+1 BB(J)=BETA GGF(J)=GGK GGM(J)=GAM TYETA(J)=ZETA IF (IEST1-GE.4.5)GJ TO 29 ARG=.707106781*ZETA CALL RATNL PYSIZ(J)=-6266570686*ZETA*EERFC PSIZZ=PPSIZ(JJ) PSIZ(JJ)=-BSIZ HJJ)=BPP TBARJ=TBARJ+FJF*GAM				170, 177
X.X(8)=1.393041				-
XXX(10)=3,302585 GN(J)=GAM2 *SRE*XX(J)*V 91 DU 1 K=1/10 G-(K)-GAM*Y(K) GAM=GN(J)+GF(K)+GAGM ODP 64 ZETA=GAM*DELTIN SIGZ=2.6±6*G*GN(J) / E(1)/GAM BETA*SIGP/SIGZ AMINDE*AVIND+1./BETA AVINDE*AVIND+1./BETA AVINDE*AVIND+1GGM*RETA AVINDE*AVIND+GM*RETA AVAQ=GAM*DSQRT((BETA*1.)/BETA) AVQ=QAM*DSQRT((BETA*1.)/BETA) AVQ=CAVQ+AAAQ CALL FH FUF=IUTZ FUF=2=10T3 1*(NUVLP-NE.0.)GU TU 6 TBARJZ=TBARJZ*FDFZ*GAM TEST1=(BETA*PSIZ)/PSIZ 1*(TEST1-GE.2.5)Gd TP 5 11=11+1 RBB(11)=BETA GGF(11)=GF(K) GGMM(11)=GAM T/ETA(J)]=ETA GGF(J)=GG(K) GGM(J)=GGM T/ETA(J)=ZETA 1*(TEST1-GE.4.5)GJ TU 29 ARG=.707106781*LETA C/LL RATNL PYSIZ(J)J=,6266573686*ZETA*EERFC PSIZZ=PPSIZ(JJ) 29 RPP=BETA*PSIZZ HJJ)=BPP 6 TBARJ=TBARJ+FJF*F*GAM			100 - 1 00 - 1	
GN(J)=GAMZ *SRE*XAX(J)*V 91 DU 1 K=1,10 GF(K)=GAM*E*Y(K) GAM=GN(J)+GF(K)+G/GM ZETA=GAM*DELTIN SIGZ=2.6±6*G*GN(J)/ E(1)/GAM BETA=SIGP/SIGZ AVIND=AVIND+1,/BETA AVIND=AVIND+6G(K)/FETA AVIND=AVIND+6G(K)/FETA AVIND=AVIND+6GM/BETA ANAQ=GAM*DSQRT((BLTA+1.)/BETA) ANAQ=AVQ+AAAQ CALL FH FJF=FUTZ FJF2=TUTZ FJF2=TUTZ FJF2=TUTZ FJF2=TUTZ GF(NUVLP-NE.O.)GU TU 6 TBARJZ=TBARJZ+FJFZ*GAM TEST1=(BETA+PSIZ)/PSIZ IF(TEST1.GE.2.5)GU TU 5 II=II+I RBB(I)=BETA GGF(I)=GF(K) GGMM(I)=GAM T/ZETA(I)=ZETA GU TU 6 JJ=JJ+1 BE(JJ)=BETA GGF(JJ)=EGTA GGF(JJ)=EGTA GGF(JJ)=GE(K) GGMMJJ=GAM T/ETA(JJ)=EGTA GGF(JJ)=EETA GCLU RATNL PPSIZ(JJ)=,6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ)=PSIZZ H\JJ)=BPP TBARJ=TBARJ+FJF*GAM			× 7 7 7 1	
911 DB 1 K=1>10 G+(K)=GAH+Y(K) GAK=GN(J)+GF(K)+GAGM ZETA=GAM*DELTIN SIGZ=2.666*G*GN(J)/ E(1)/GAM BETA=SIGP/SIGZ AVIND=AVIND+1,/BETA AVINDE=AVIND+6F(K)/FETA AVINDT=AVIND+6F(K)/FETA AVINDT=AVIND+GAM/BETA AAAQ=GAM*DSQRT((B:TA+1.)/BETA) AOQ=AVQ+AAAQ CALL FH FJF=IUT2 GJF2=TOT3 IF(NUVLP.NE.0.)GU TU 6 TBARJ2=TBARJ2+FJP2*GAM TFST1=(BETA+PSIZ)/PSIZ I+(TEST1.GE.2.5)GU TD 5 II=II+1 BBB(II)=BETA GGFF(II)=GFK) GGMM(I)=GAM TIZETA(II)=ZETA GGF(II)=GFK) GGM(JJ)=GAM TYETA(JJ)=EETA GGF(JJ)=GFK) GGM(JJ)=GAM TYETA(JJ)=EETA GGF(JJ)=GFK) GGM(JJ)=GAM TYETA(JJ)=BETA TYETA(JJ) TY			DOP	60
GF(K)=Gff+*Y(K) GAM=GN(J)+GF(K)+GAGM CDP 64 ZETA=GAM*DELTIN SIGZ=2.6.6*G*KGN(J)/ E(1)/GAM BETA=SIGP/SIGZ AMIND=AVIND+1./BETA AVINDF=AVIND+GF(K)/EETA AVINDT=AVIND+GF(K)/EETA AVINDT=AVINDT+GAM/BETA AAAQ=GAM*DSQRT((BETA+1.)/BETA) AAQ=QAM*DSQRT((BETA+1.)/BETA) AAQ=QAM*DSQRT((BETA+1.)/BETA) AAQ=QAM*DSQRT((BETA+1.)/BETA) AFFICUT2 GFZ=TOT3 IF(NOVLP.NE.O.)GO TO 6 TBAR J2=TBARJ2+FJ2*GAM TEST1=(BETA+PSIZ)/PSIZ 1F(TEST1.GE.2.5)GO TO 5 Ii=II+1 BBB(II)=BETA GGF(II)=GF(K) GGMM(II)=GAM TIZETA(II)=ZETA GU TO 6 JJ=JJ+1 BB(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TO 29 ARG=.707106781*ZETA CALL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ(ZJD)=PSIZ(JJ) PPPBETA+PSIZ2 PPSIZ(JJ)=PSIZ(JJ) PPPBETA+PSIZ2 PPSIZ(JJ)=PSIZ H(JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM	011			
GAM=GN(J)+GF(K)+GAGM ZETA=GAM*DELTIN SIGC=2.6c6*C*GN(J)/ E(1)/GAM BETA=SIGP/SIGZ AVIND=AVIND+1./BETA AVINDF=AVINDF+GF(K)/EETA AVINDF=AVINDF+GF(K)/EETA AVINDT=AVINDT+GAM/BETA A^AQ=GAM*DSQRT((BETA+1.)/BETA) A^Q=AVQ+AAAQ CALL FH FJF=FIDT2 FJF=FIDT2 FJF=FIDT3 IF (NUVLP-NE-0.)GU TU 6 TBAM J2=TBAR J2+FJH-2*GAM TEST1=(BETA+PSIZ)/PSIZ IF (TEST1-GE.2.5)GU TU 5 Ii=II+1 BAB(II)=BETA GGFF(II)=GF(K) GGMM(II)=GAM TIZETA(II)=ZETA GU TU 6 5 JJ=JJ+1 BB(JJ)=GAM T/ETA(JJ)=ZETA IF (TEST1-GE.4.5)GJ TU 29 ARG=.707106781*ZETA CALL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ(Z=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ H(JJ)=BPP 6 TBAR J=FBARJ+FJF*GAM	911		OUB	63
SIGZ=2.666%G*GN(J)/ E(1)/GAM BETA*SIGYSIGZ AMIND=AVIND+1./BETA AVINDF=AVIND+6F(K)/EETA AVINDT=AVINDT+GAM/BETA ANAQ=GAM*DSQRT((B_TA+1.)/BETA) AVQ=AVQ+AAAQ CALL FH FJF=TDT2 FJF2=TDT3 IF(NDVLP.NE.O.)GO TO 6 TBARJ2=TBARJ2+FJF2*GAM TEST1=(BETA+PSIZ)/PSIZ IF(TEST1.GE.2.5)GO TO 5 II=II+1 BBB(II)=BETA GGFF(II)=GF(K) GGMM(II)=GAM TZETA(II)=ZETA GGF(JJ)=GF(K) GGM(JJ)=GAM TZETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TO 29 ARG=.707106781*ZETA CALL RATNL PPSIZ(JJ)=BPSIZ(JJ) PPSIZ(JJ)=PSIZZ PPSIZ(JJ)=PSIZZ PSIZ(JJ)=PSIZZ PSIZ(JJ)=PSIZZ H(JJ)=BPP TBARJ=TBARJ+FJF*GAM				
BETA=SIGP/SIGZ AVIND=AVINDH+GF(K)/EETA AVINDE=AVINDH+GF(K)/EETA AVINDE=AVINDH+GF(K)/EETA AVINDT=AVINDH+GAM/BETA ANAQ=CAMMDSQRT((B_TA+1.)/BETA) AVQ=AVQ+AAAQ CALL FH FJF=TDT2 FJF2=TDT3 IF (NUVLP.NE.O.)GO TO 6 TBARJ2=TBARJ2+FJF2*GAM TEST1=(BETA+PSIZ)/PSIZ IF (TEST1.GE.2.5)GO TO 5 II=II+1 BBB(I)=BETA GGFF(11)=GF(K) GGMM(I1)=CAM TIZETA(I1)=ZETA GB TU 6 JJ=JJ+1 BB(J)=BETA GGF(JJ)=GF(K) GGM(J)=GAM T/ETA(JJ)=ZETA IF (TEST1.GE.4.5)GJ TO 29 ARG=.707106781*ZETA C/LL RATNL PSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ(JJ)=PSIZ(JJ) PSPIZ(JJ)=PSIZ PSIZ(JJ)=PSIZ H(JJ)=BPP TBARJ=TBARJ+FJF*GAM				
AVIND=AVIND+1,/BETA AVINDT=AVIND+FG(K)/EETA AVINDT=AVIND+GG(K)/EETA AVINDT=AVIND+GGM/BETA A^AQ=GAM*DSQRT((BLTA+1.)/BETA) A^Q=AVQ+AAAQ CALL FH FJF=IOT2 GJF2=TOT3 IF(NOVLP.NE.O.)GO TO 6 TBARQ2=TBARQ2+FJ+2*GAM TEST1=(BETA+PSIZ)/PSIZ IF(TEST1.GE.2.5)GO TO 5 II=II+1 BBB(II)=BETA GGFF(II)=GF(K) GGMM(II)=GAM TIZETA(II)=ZETA GU TO 6 JJ=JJ+1 BB(JJ)=BETA GGF(JJ)=GE(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TO 29 ARG=.707106781*ZETA CLL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ(JJ)=PSIZ(JJ) 29 BPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H(JJ)=BPP 6 TBARJ=TBARQ1+FJF*GAM				47
AVINDF=AVINDF+GF(K)/PETA AVINDT=AVINDT+GAM/BETA AAAQ=GAM*DSQRT((BETA+1.)/BETA) AVQ=AVQ+AAAQ CALL FH FJF=IUT2 FJF2=TOT3 IF(NOVLP.NE.O.)GO TO 6 TBARJ2=TBARJ2+FJF2*GAM TEST1=(BETA+PSIZ)/PSIZ IF(TEST1.GE.2.5)GO TO 5 I1=II+1 RBB(II)=BETA GGFF(II)=GF(K) GGMM(II)=GAM TTZETA(II)=7ETA GB TO 6 JJ=JJ+1 BB(JJ)=BETA GGF(JJ)=BETA GGF(JJ)=CAM TZETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TO 29 ARG=.707106781*ZETA LF(TEST1.GE.4.5)GJ TO 29 ARG=.707106781*ZETA PSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ(JJ)=PSIZ(JJ) 29 RPP=BETA+PSIZ2 PSIZ(JJ)=PSIZ H(JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM			9012	0/
A^AQ=GAM*DSQRT((B:TA+1.)/BETA) A^Q=AVQ+AAAQ C^ALL FH FUF=FUT2 FUF=TUT3 If(NUVLP.NE.O.)GU TU 6 TBARJ2=TBARJ2+FUF2*GAM TEST1=(BETA+PSIZ)/PSIZ If(TEST1.GE.2.5)GU TU 5 Ii=II+1 BAB(I)=BETA GGFF(II)=GF(K) GGMM(II)=GAM TIZETA(II)=ZETA GU TU 6 JU=JJ+1 BB(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TU 29 ARC=.707106781*ZETA C/LL RATNL PFSIZ(JJ)=.6266570686*ZETA*EERFU PSIZ(PPSIZ(JJ)=PSIZ2 PPSIZ(JJ)=PSIZ2 HJJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
A*Q=AVQ+AAAQ CALL FH FUF=FUT2 #JF2=TUT3 I*(NUVLP=NE.O.)GU TU 6 TBARJ2=TBARJ2+FJF2*GAM TEST1=(BETA+PSIZ)/PSIZ I*(TEST1.GE.2.5)GU TU 5 I!=II+1 B*B*Q[I]=BETA GGFF(II)=GF(K) GGMM(II)=GAM TIZETA(II)=ZETA GU TU 6 5 JU=JJ+1 B*C(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA GF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA I*(TEST1.GE.4.5)GJ TU 29 A*RC=.707106781*ZEFA C/LL RATNL P*SIZ(JJ)=.6266570686*ZETA*EERFC P*SIZ2=PPSIZ(JJ) 29 *R*P=BETA+PSIZ2 P*SIZ(JJ)=PSIZ2 H*JJJ=BPP T*BARJ=TBARJ+FJF*GAM		AVINDT=AVINDT+GAM/8ETA		
CALL FH FJFFTOT2 FJF2=TOT3 IF(NOVLP-NE.O.)GO TO 6 TBARJ2=TBARJ2+FJF2*GAM TEST1=(BETA+PSIZ)/PSIZ IF(TEST1.GE.2.5)GO TO 5 II=II+1 BBB(II)=BETA GGFF(II)=GF(K) GGMM(II)=GAM TIZETA(II)=ZETA GU TO 6 JJ=JJ+1 BB(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TO 29 ARG=.707106781*ZETA CALL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFO PSIZ2=PPSIZ(JJ) 29 BPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H\JJ)=BPP TBARJ=TBARJ+FJF*GAM				
FJF=TOT2 #JF=TOT3 IF (NOVLP-NE.O.)GO TO 6 TBARJ2=TBARJ2+FJF2*GAM TEST1=(BETA+PSIZ)/PSIZ IF (TEST1.GE.2.5)GO TO 5 II=II+1 ### ### ### ### ### ### ### ### ### #				
#JF2=TOT9 IF (NOVLP-NE.O.)GU TU 6 TBARJ2=TBARJ2+FJ+2*GAM TEST1=(BETA+PSIZ)/PS1Z IF(TEST1-GE.2.5)GU TU 5 Ii=II+1 BBB(II)=BETA GGFF(11)=GF(K) GGMM(II)=GAM TTZETA(II)=ZETA GU TU 6 JJ=JJ+1 BB(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1-GE.4.5)GJ TU 29 ARG=.707106781*4EFA C/LL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H(JJ)=BPP TBARJ=TBARJ+FJF*GAM				
TBARJ2=TBARJ2+FJF2*GAM TEST1=(BETA+PSIZ)/PSIZ IF(TEST1.GE.2.5)Gd TD 5 I1=II+1 BBB(II)=BETA GGFF(II)=GF(K) GGMM(II)=GAM TIZETA(II)=ZETA GU TU 6 JU=JJ+1 BB(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TU 29 ARG=.707106781*ZETA CALL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ(JJ)=PSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ H\JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
TEST1=(BETA+PSIZ)/PSIZ 1F(TEST1.GE.2.5)GO TO 5 1i=II+1 BBB(II)=BETA GGFF(II)=GF(K) GGMM(II)=GAM TTZETA(II)=ZETA GU TU 6 5 JU=JJ+1 BB(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM TZETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TO 29 ARG=.707106781*ZETA CZLL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ(ZJ)=PSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZZ H\JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
1F(TEST1.GE.2.5)GO TO 5 II=II+1 BBB(II)=BETA GGFF(II)=GF(K) GGMM(II)=GAM TIZETA(II)=ZETA GB TU 6 5 JU=JJ+1 BB(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TO 29 ARG=.707106781*ZETA C/LL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H(JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
II=II+1 888(II)=BETA GGFF(11)=GF(K) GGMM(II)=GAM TTZETA(II)=ZETA GU TU 6 JJJ=JJ+1 88(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM TZETA(JJ)=ZETA IF(TEST1-GE-4-5)GJ TU 29 ARG=-707106781*ZETA CZUL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) PPSIZ(JJ)=PSIZ2 PPSIZ(JJ)=PSIZ2 H(JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
GGFF(II)=GF(K) GGMM(II)=GAM TTZETA(II)=ZETA GU TU 6 JJ=JJ+1 BB(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TESTI-GE-4-5)GJ TU 29 ARG=.707106781*/ETA CALL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) PPPBETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H(JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
GGMM(II) = GAM TIZETA(II) = ZETA GU TU 6 5 J = JJ + 1 BB(JJ) = BETA GGF(JJ) = GF(K) GGM(JJ) = GAM T/ETA(JJ) = ZETA IF(TESTI - GE - 4 - 5) GJ TU 29 ARG = . 707106781 * ZETA CALL RATNL PPSIZ(JJ) = .6266570686 * ZETA * EERFC PSIZ2 = PPSIZ(JJ) 29 RPP = BETA + PSIZ2 PPSIZ(JJ) = PSIZ2 H(JJ) = BPP 6 TBARJ = TBARJ + FJF * GAM		BBB(II)=BETA		
TIZETA(I1)=ZETA GU TU 6 5 JU=JJ+1 BB(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM TZETA(JJ)=ZETA IH(TEST1.GE.4.5)GJ TU 29 ARG=.707106781*ZETA CALL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H\JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
GU TU 6 5 JU=JJ+1 BB(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TU 29 ARG=.707106781*ZETA C/LL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H(JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
B&(JJ)=BETA GGF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TU 29 ARG=.707106781*/ETA C/LL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H\JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
GGF(JJ)=GF(K) GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TD 29 ARG=.707106781*/ETA C/LL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 PPSIZ(JJ)=PSIZ2 H(JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM	5			
GGM(JJ)=GAM T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TD 29 ARG=.707106781*/ETA C/LL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H(JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
T/ETA(JJ)=ZETA IF(TEST1.GE.4.5)GJ TU 29 ARG=.707106781*4ETA C/LL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H\JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
IF(TEST1.6E.4.5)GJ TO 29 ARG=.707106781*4ETA CALL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H(JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
CALL RATNL PPSIZ(JJ)=.6266570686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H\JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM		IF (TEST1.GE.4.5)GJ TO 29		
PPSIZ(JJ)=.6266573686*ZETA*EERFC PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H\JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
PSIZ2=PPSIZ(JJ) 29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H\JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM		C/LL RAINL DUST7(11) = .6266570686*7FTA*FFRFC		
29 RPP=BETA+PSIZ2 PPSIZ(JJ)=PSIZ2 H\JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM				
PPSIZ(JJ)=PSIZ2 H(JJ)=BPP 6 TBARJ=TBARJ+FJF*GAM	29	RPP=BETA+PSIZ2		
6 TBARJ=TBARJ+FJF*GAM		PPSIZ(JJ)=PS1Z2		
BARJ=BARJ+FJF	,	HIJJ)=BPP		
UNIV PRICE STATE	0	RAD I=BARJ+FJF	DOP	73

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A-3
  1 GFBARJ=GFBARJ+FJF*GF(K)
                                                                            POC
   BARJ=.01*BARJ*GMGM/D
    GFBARJ=. 01*GFBARJ/D
    THARJ=.01*TBARJ/D
    IH (NOVLP.NE.O.) 60 TO 709
    AVQ = . 01 * AVQ
    AVIND=.01570796327*AVIND*GMGM/D
    PRINT 730, AVIND, AVO
730 FURMAT (7H AVIND=012.5,5H AVQ=012.5)
    A'GABB = AVG
    PRINT 51, AVGABB
 51 FURMAT(8H AVGABB=012.5)
    PRINT 8, II.JJ
  8 FURMAT (4H II=16,4H JJ=16)
    TZ=TLEFT(DD)
    T!J=(T1-12)*.01
    T3=TLEFT(00)
    BARING=AVIND
    BARINF = . 01570796327*AVINDF/D
    BARINI = . 01570796327*AVINOT/D
    TPARJ2=.01*TBARJ2/D
    DZ=TBAR.12
    SEG=(BARING-BARI) *DZ
    SEF=(BARINF-GFBARJ)*02
    SET=(BARINT-TBARJ)*12
    PRINT 9151, SEG, SEF, SET, D2
9151 FURMAT (6612.5)
    ALP=USQRT(.5/DELTin**2+(1/*.318309)**2+AVGABB**2)
    DU 36 N=1,5
    SI(N)=DABS(YY(N)/ALP)
    ARG1=SI(N)
    E4(N)=DEXP(.5*(.5*ARG1/DELTIN) **2)
    E2(N)=E4(N)*E4(N)
    E1(N)=E3(N)/(E2(N)*E2(N))
    E1(N+5)=E1(N)
    E2(N+5)=E2(N)
    E3(N+5)=E3(N)
 36 CONTINUE
    IF (II.EQ.O)GO TL
    DU 33 J=1, II
    DU 11 N=1,5
    ARGI=SI(N)
    B(N, J)=1.2533156*DEXP(-.5*GGMM(J)*ARG1)
    ANDRM(N) = E2(N) * (BBB(J) + NW(N) * E3(N) * . 25 * GGMM(J) / ALP)
    BP(N,1)=B(N,J)/ANJRM(N)
    3P(N+5,1)=BP(N,1)
    ANDRM(N+5) = ANDRM(N)
   DU 11 K=1,10
    IF (N.EQ.K) GU TO 110
    A(N,K)=.25*WW(K)*E1(K)*DEXP(.5*(1./DELTIN/ALP)**2*YY(N)*YY(K)-
   XDABS(YY(N)=YY(K)) *.5*GGMM(J)/ALP)/ALP/ANDRM(N)*E2(K)*GGMM(J)
    GO TO 111
110 A(N,K)=1.
111 1 + (K.GT.5)GD TO 112
    S(NoK) = A(NoK)
   DUM5 (NoK) = A(NoK)
   GL TU 11
112 DUM1 (N,K-5) = A(N,K)
11 CONTINUE
   CALL MATRIX(5, DETERM, 5)
```

74

```
UU 72 M=1,2
   DU 93 L=1,5
   DUM3 (M, L) = 0.
   DU 92 N=1,5
   DUM2 (N, 1) = 0.
   DU 91 K=1,5
91 DUM2 (N, L) = DUM2 (N, L) + S (N, K) * DUM1 (K, L)
92 DUM3 (M, L) = DUM3 (M, L) + DUM1 (M, N) * DUM2 (N, L)
   DUM4 (M, L) = DUM5 (M, L) - DUM3 (M, L)
93 CUNTINUE
   CALL MATRIX(DUM4, DETERM, 5)
   DU 73 M=1,5
   VECT (M. 1) = 0.
   DU 75 N=1,10
   17 (N.GT.5) GU TO 74
   VECT (M, 1) = VECT (M, 1) + 0UM4 (M, N) * 8P (N, 1)
   DUM6 (M, N) = 0.
   DU 71 K=1,5
71 DUM6(M, N) = DUM6(M, N) + DUM2(M, K) * DUM4(K, N)
   DUM1 (M, N+5) = - DUM6 (M, N)
   GU TU 75
74 VECT (M, 1) = VECT (M, 1) + DUM1 (M, N) *BP(N, 1)
75 CUNTINUE
   DUMMY (M, J) = VECT (M, 1)
73 CUNTINUE
   DU 76 M=1.5
   VECT2(M)=0.
   DU 77 N=1,10
   IF (N.GT.5)GD TO 73
   VECT2(M)=VECT2(M) +DUM4(M,N)*VECT(N,1)*E2(N)*BBB(J)/ANDRM(N)
   GO TO 77
78 VECT2(M)=VECT2(M) +DUM1(M,N)*VECT(N-5,1)*E2(N)*BBB(J)/ANDRM(N)
77 CUNTINUE
   DUMMY2(M)J)=VECT2(M)
76 CUNTINUE
33 CUNTINUE
   DU 34 N=1,5
   AVGGMT(N)=0.
   AVGFMT(N)=0.
   AVGIMT(N)=0.
   AVT1(N)=0.
   RING(N)=U.
   BINF(N)=0.
   BINT(M)=0.
   DU 34 J=1, 11
   AVGGMT(N) = AVGGMT(N) + DUMAY(N, J) *E2(N)
   AVGEMT(N) = AVGEMT(N) + DUMMY(N, J) *E2(N) *GGFF(J)
   AVGTMT(N)=AVGTMT(N)+DUMMY(N,J)*E2(N)*GGMM(J)
   BING(N) = BING(N) + B(N, J) / BBB(J)
   BINF(N)=BINF(N)+B(N,J)*GGFF(J)/BBB(J)
   BINT(N)=BINT(N)+B(N,J)*GGMM(J)/BBB(J)
   AVT1(N)=AVT1(N)+DUMMY2(N,J)*E2(N)*GGMM(J)
34 CONTINUE
7 DU 3333 M=1,5
  AVGG=O.
   AVGF=0.
   AVGT=Q.
  AVTQZ=0.
  AVGQZ=0.
  AVFQZ=0.
```

```
IF (JJ.EQ.O)GO TO 9
    AKG1=SI(M)
    QQ=D*ARG1/3.1410
    DUM= . 5 * ARG1/DEL TIN/1. 4142
    ARG = DUM
    CALL RAINL
    AL=E4(M)-EERFC
    0=1.
    AL 333 J=1,JJ
    TEST6= H(J)/PPSIZ(J)
    IF (TEST6.GE.25.)G: TH 223
    ARG=DUM+TZETA(J)/1.4142
    CALL RATNL
    AZ=EERFC
    1= .626658*TZETA(J)*(A1+A2)
    Q=1.+(PPSIZ(J)-U)/H(J)
    02=(H(J)/3B(J))-0
    Q3=(Q-.5)*2.*BB(J)/H(J)
223 EE1=DEXP(-.5*GGM(J)*ARG1)/H(J)
    AVGG=AVGG+EE1*Q
    AVGF=AVGF+GGF(J)*Q*EE1
    AVGT=AVGI+GGM(J) *Q*EE1
    IF (TEST6.GE.25.) GO 10 333
    AVGQZ=AVGQZ+QZ*EE1
    AVFQ2=AVFQ2+Q2*EE1*GGF(J)
    AVTQ2=AVTQ2+Q2*EE1*GGM(J)
    AVT03=AVT03+03*EE1*GGM(J)
 333 CUNTINUE
    IF(II.GT.O)GD TE 9
    AVGGMT (M) = 0.
    AVGFMT(M)=0.
    AVGIMT(M)=0.
    BING(M)=0.
    BINF(M)=0.
    BINT (M) = 0.
    AVT1(M)=0.
  9 DVLG=.01*(AVGG+AVGGMT(M)*.7978836)*GMGM
    DVLF=.01*(AVGF+AVGFMT(M)*.7978836)
    DVLT=.01*(AVGT+AVGTMT(M)*.7978836)
    DVLG2=.01*(AVGQ2+ .7978836*(BING(M)-AVGGMT(M)))*GMGM
    DVLF2=.U1*(AVFQ2+.7978836*(BINF(M)-AVGFMT(M)))
    DVLT2=.01*(AVTQ2+.7978836*(BINT(M)-AVGTMT(M)))
    DVLT3=.01*(AVTQ3+.7978836*AVT1(11))
894 IF (QQ.GT.2.)GU TO 498
    FDYSON=(1.-00+.5*00*DLOG(1.+00))
    GL TU 933
498 FDYSUN=.5*QQ*DLUG((1.+QQ)/(QQ-1.))-1.
933 DUM=WW(M) * OVLT*FDYSON*E1(M) *2./D
    FG=FG+UVLG*DUM
    FF=FF+OVLF*DUM
    FI=FT+NVLT*DUM
    DUMM=WW(M) +DVLT3 +FDYSDN +E1(M) +2./D
    FG2=FG2+DUMM*DVLG2
    FF2=FF2+DUMM*UVLF2
    FIZ=F12+DUMN*UVLT2
3333 CUNTINUE
    DVFRLG=(+G-FG2)*.3927/ALP
```

OVERLE=(FF-FF2)*.3927/ALP
OVERLT=(FT-FT2)*.3927/ALP

DOP

```
DYG=BARJTTBARJ-SEG=OVERLG
   OVF=GFBARJ*TBARJ-SEF-DVERLF
   DVT=TBARJ*TBARJ-SET-UVERLT
   PRINT 9151, FG, FG2, OVERLG, FF, FF2, OVERLF
    IF (UVG.GT.0.) 57 TO 14
709 DYG=0.
    TVF=0.
   DVT=0.
14 PRINT 701, DVG, DVF, OVT
701 FURMAT (SH DVG=D12.5,5H UVF=D12.5,5H DVT=D12.5)
   PRINT 702, BARJ, GFBARJ, TBARJ
702 FURMAT (6H BARJ=E12.5,8H GFBARJ=E12.5,7H TBARJ=E12.5)
   UNRGM(I) = UNRGM(I) + SIGP * BARJ
    T4=TLEFT(DD)
    TID=(T3-14)*.01
    PRINT 13, TTJ, TTO
13 FORMAT(5H TTJ=E12.5,5H (TO=E12.5)
   MARG(I) = UNRG(I) + SIGP * GFBARJ
    FLUXCT(I)=1.-(TBARJ-DVT)
   CAP(1)=CAP(I)+SIGP*(BARJ-DVG)/FLUXCT(I)
    FISS(I)=FISS(I)+SIGP*(GFBARJ-OVF)/FLUXCI(I)
  2 CUNTINUE
   RETURN
   END
    SUBRUUTINE FH
    IMPLICIT REAL *8 (4-H, D-Z)
    COMMON/TRTI/12(62,62), TI(62,62), AIMW, AX, REW, WHY, KI
   CUMMUN/H/TEST1, TEST2, HH
   CUMMUN /QFJ1/ZETA, TOTZ, BETA, PSIZ, PSIZ2, PS3
   CUMMON/R/ EERFC, ARG
   CLIMMUN/F/AKI, DEN, RAT, C, AAA
   CUMMON/SEC/TUT3, TUT4
   DIMENSION ZLP(B)
   DIMENSION RAT(10), AKI(10), DEN(10)
   DIMENSION ALP(5)
   DIMENSION AN(10) PM(10)
   DATA AN/ .1666667, .33333333D-1, .7142857D-2, .1587302D-2,
  X.3607504D-3,.8325008D-4/
   DATA BM/.1666667,.55555550-1,.12345680-1,.20576130-2,
  X.2743484U-3,.3048316D-4/
   DATA ALP/.9848077530,.8060254038,.6427876097,.3420201433/
   DITA ZLP/
                  .2393156642,.4647231720,.6631226582,.8229838658,
  X.9350162426, .9927088740/
   K1=1
   WHY= . 5 * ZETA
   ARG=WHY
   CALL RAINL
   PSIZ=.8862269*ZETA*EERFC
   H=RETA+PSIZ
   TESTI=H/PSIZ
   AINTZ=.5/TEST1
   ASO=AAA**2
   IF (TEST1.GE.15.) GO TO 100
   IF (ZETA. GT. 2.5) 60 TO 20
   1+ (TEST1.GE.4.5) GI TO 100
   TF (BETA. GE . . 018) GJ TD 2
   IF (ZETA.GE.. 5) GU TO 20
   BUVPSI=BETA/PSIZ
   IF (BUVPSI.GE .. 2) GO TO 2
   RH=4.*(1.8971+DLOG(1.+./532929*ZETA/BETA))/ZETA**2
```

A- 6

DOP

DOP

DOP

DOP

DOP

DOP

```
TEST2=BB*BETA
   IF (TEST2.GT..03) GU TO 4
   GU TU 20
 2 C=5./ZETA
   GU TU 3
 4 1 (TEST2.LT.1.0) GD TU 11
   FAC=1.+.018*(BFTA-.00128)/(BETA+.00128)+.08*BDVPSI
   C=.8292*DSQR1( 68)*FAC
   GU TU 3
11 C=.7071*DSQRT(BB+(1.+BETA)/BETA)
 3 TUT2=0.
   TUT3=0.
   TUT4=0.
   DO 1 1=1,6
   AX=WHY*ZLP(1)*C/DSQRT(1.-ZLP(1)**2)
   CALL QUICKW
   PSI=.8862269*/ETA*REW
   AKI(1) = . 8862269 * ZETA * AIMW
   DEN(I)=BETA+PSI
   RAT(1)=PSI/DEN(1)/(1.-ZLP(1)**2)
   TOT3=TOT3+RAI(I)*BETA/DEN(I)
   AKISQ=AKI(I)**Z*ASQ
   TUT4=TUT4+(AKISQ/(DEN(I)**2-AKISQ))*RAT(I)
 1 TUT2=TUT2+RAT(I)
   TUT2=TOT2+AINTZ
   TUT2=TUT2*C*.2416609733
   TUT3=TOT3+AINTZ*(1.-1./TEST1)
    TUT3=TUT3*C*.2416609733
   TOT4=TUT4*C*.2416609733
   RETURN
100 ARG= . 707106781*ZETA
   CALL RATNL
   PS122=.6266570686*ZETA*EERFC
   HH=BETA+PSIZ2
   10T2=1.57079632681/HH
   TUT3=TUT2*BETA/HH
   Z=ZETA*ZETA
   IF (ZETA.GT.2.5)GD TD 23
   ARG= . 40824829*ZETA
   CALL RAINL
   PS1Z3=.7236021*ZEIA*EERFC
   5=0.
   SUM = 0 .
   TEMP=1.
   DC 22 I=1,6
   TEMP=TEMP*Z
   SUM=SUM+BM(1) *TEMP
   S=S+AN(1)*(SUM+.25)
22 CUNTINUE
   5=5+.25
   ZEX=2.1708037*ZETA*DEXP(Z/6.)
   PS3=(PS1Z2*(3.*PS1Z3-ZEX)+1.5*Z*S)*1.5707963281
   GI TO 24
23 TAUTHZ = . 66666667*Z
   El=(IWDTHZ*(IWDTHZ+2.334733)+.250621)/(TWDTHZ*(TWDTHZ+3.330657)+
  X1.681534)
   H1=1 .- E1
   H2=1.5/Z-H1
   H3=5./(Z*Z)-1.11111111+H2
   H4=26.25/(Z*Z*Z)-1.1666567*H3
```

```
PS3=.58904862*E1-(H1-H2+H3-H4)*.39269908
24 TUT4=.3333333*ASQ*PS3/(HH*HH*HH)
   IF (TEST1.LT.15.) GO TO 33
   RETURN
33 TUT2=1012+(PS3-PS1Z2*PSIZ2*1.5707963281)/(HH*HH*HH)
   TUT3=TUT3*(1.+3.*(.6366132837*PS3-PSIZ2*PSIZ2)/(HH*HH))
   TUT4=.33333333*ASQ*PS3/(HH*HH*HH)
   RETURN
20 C=. 7171*DSQRT((1.+BETA)/BETA)
   TTTZ=0.
   T.173=0.
   TUT4=0.
   NU 9 1=1,4
   AX=WHY*ALP(1)*C/DSQRT(1.-ALP(1)**2)
   CALL QUICKW
   PSI=.8862269*ZETA*REW
   AKI(1)=.8862269*ZETA*AIMW
   DEN(I)=BETA+PSI
   RAT(1) = PSI/DEN(1)/(1.-ALP(1)**2)
   TUT3=TUT3+RAT(I)*BETA/DEN(I)
   AK I SQ = AK 1 ( 1 ) ** 2 * ASQ
   TUT4=TUT4+(AKISQ/(DEN(I)**2-AKISQ))*RAT(I)
 9 TUT2=1012+RAT(1)
   TUTZ=TOTZ+AINTZ
   TUT2=TUT2*C*.3490558504
   TUT3=TUT3+AINTZ*(1.-1./TEST1)
   TOT3=TOT3*C*.3490658504
   TUT4=TOT4*C*.3490058504
   RETURN
```

END

